# NUMERICAL MODELLING OF THE GEOCHEMICAL EVOLUTION OF THE NEAR FIELD UNDER THE HYDROTHERMAL CONDITIONS EXPECTED FOR A KBS-3 REPOSITORY

**D. Arcos[1], C. Sena[1], J. Salas[1]**

**1. Amphos XXI Consulting S.L., Barcelona, Spain (david.arcos@amphos21.com)**

In the KBS-3 concept for the nuclear waste repository, designed by the Swedish Nuclear Fuel and Waste Management Co. (SKB), the bentonite buffer is placed around the copper canisters that contain the spent nuclear fuel, isolating it of the host rock. In order to check – hypotheses for the evolution of the bentonite buffer under the thermo-hydraulic conditions expected in a KBS-3 repository, SKB is conducting a series of long term buffer material (LOT) tests at the Äspö Hard Rock Laboratory (HRL).

In the present work, numerical simulations are developed to simulate:

i) thermo-hydraulic processes;

ii) geochemical reactions and;

iii) transport of solutes,

that have been measured in the LOT A2 test (Karnland *et al.*, 2008), and, that are expected in the near-field of a KBS-3 repository.

The numerical model for the LOT A2 test is based on analytical results (Villar *et al.*, 2008) and on field-scale experiments (Karnland *et al.*, 2008). The validation of this model allows us to implement it for the thermal period of the near field of the KBS-3 repository, based on previous modelling exercises (Arcos *et al.*, 2003; Arcos *et al.*, 2008).

During the operation of a KBS-3 repository (after deposition of the copper canisters), the unsaturated bentonite will be submitted to a relatively high thermal gradient, induced by the radioactive decay of the spent nuclear fuel. On the other hand, the saturated host rock will provide aqueous solution to the unsaturated bentonite, induced by differential hydraulic pressures, under specific thermal and mechanic conditions. In this context, the bentonite will gradually become fully water saturated. Experimental results (Karnland *et al.*, 2008) indicate that during the saturation period, the transport of solutes in the bentonite buffer will be influenced by water uptake from the surrounding host rock towards the wetting front, and also by a cyclic evaporation/condensation process, induced by the thermal gradient (Figure 1).

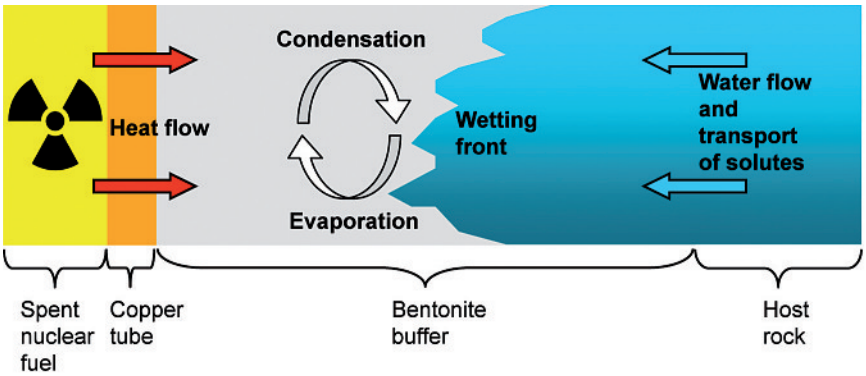


**Figure 1:** Vertical cross section of the near-field of a KBS-3 repository showing the thermo-hydraulic and transport processes that are believed to occur during the saturation period of the bentonite buffer.

Our numerical models take into account the transport of solutes and geochemical reactions under non-isothermal conditions, and in a scenario of variable pore water saturation. The reference groundwater composition that represents the host rock groundwater (mainly located in fractures) is taken from a borehole drilled in the Äspö HRL that supplied the LOT A2 test. The initial pore water composition of the bentonite buffer is based on the experimental results attained in Karnland *et al.* (2008).

From the mineralogical description of the MX-80 bentonite, and under the pH and redox conditions expected for the near-field of the future KBS-3 repository, the main reactive minerals of the bentonite buffer are montmorillonite, gypsum and pyrite. In terms of its solubility, montmorillonite seems to remain relatively stable under the geochemical and thermo-hydraulic conditions of a KBS-3 repository (Karnland *et al.*, 2008), and therefore, it only participates in cation exchange reactions. Finally, from the results attained in previous works (Arcos *et al.*, 2008; Karnland *et al.*, 2008), anhydrite and calcite are let to precipitate if oversaturation is reached.

The numerical model developed for the LOT A2 test indicates that the bentonite buffer is fully water saturated within the first half-year which is in agreement with measured data (Figure 2).

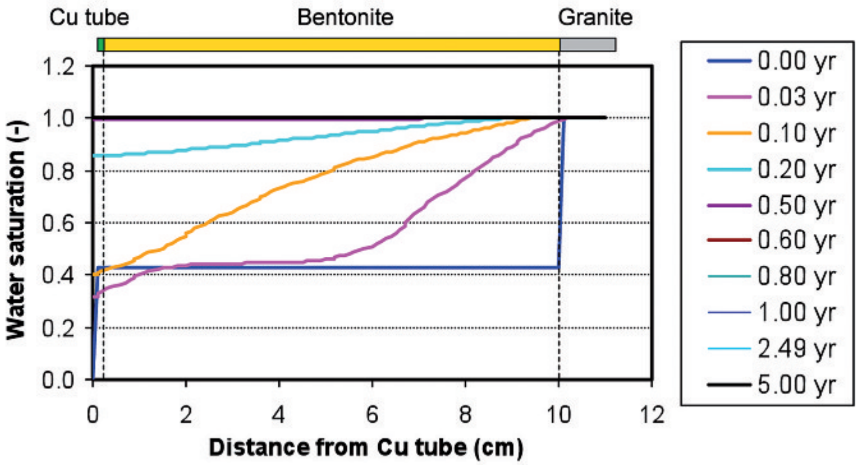


**Figure 2:** Computed evolution of the saturation of the bentonite blocks located at the depth of the heater of the LOT A2 test.

Numerical results indicate that, despite the evaporation/condensation cycling, the chloride transported by the flow of Äspö groundwater into the bentonite buffer behaves conservatively (no chloride salts precipitate). In addition, numerical results indicate that the behaviour of anhydrite, gypsum and calcite is influenced by the thermal gradient that is established during the saturation period of the bentonite buffer.

**References:**

Arcos, D., Bruno, J., Karnland, O., 2003. Geochemical model of the granite-bentonite-groundwater interaction at Äspö HRL (LOT experiment). *Applied Clay Science*, 23: 219-228.

Arcos, D., Grandia, F., Domènech, C., Fernández, A.M., Villar, M.V., Muurinen, A., Carlsson, T., Sellin, P., Hernán, P., 2008. Long-term geochemical evolution of the near field repository: Insights from reactive transport modelling and experimental evidences. *Journal of Contaminant Hydrology*, 102: 196-209.

Karnland, O., Olsson, S., Dueck, A., Birgersson, M., Nilsson, U., Heman-Hakansson, T., 2008. *Long-term test of buffer material – Parcel A2 field and laboratory draft report*. SKB report.

Villar, M.V., Sánchez, M., Gens, A., 2008. Behaviour of a bentonite barrier in the laboratory: Experimental results up to 8 years and numerical simulation. *Physics and chemistry of the Earth*, 33: S476-S485.